Reaction Pathway Analysis for metal catalyzed Fischer Tropsch Synthesis

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In the framework of a circular economy Fischer Tropsch Synthesis (FTS) is considered as attractive reaction to produce light olefins (C2-C4) from syngas generated via gasification of plastics [1] . In general FTS takes place on a transition metal (cobalt, iron) at moderate to high pressures and elevated temperatures, where the hydrogenation of carbon monoxide occurs to produce key building blocks for chemical industry. It occurs via a multitude of elementary steps, correspondingly requiring a large number of kinetic parameters for simulation Purposes.

The Single Event Micro -Kinetic methodology (SEMK) can be used to classify the large number of elementary steps into a limited number of reaction families and hence reduce the number of kinetic parameters in the model [2],[3].Thus, SEMK models can be applied in commercial reactor design. Furthermore, and by incorporating so called catalytic descriptors in the model, SEMK can likewise be used for rational catalyst design. In this respect reaction pathway analysis (RPA) serves as an important tool to analyze the occurring phenomena, elementary steps both in a qualitative and quantitative manner.[3].

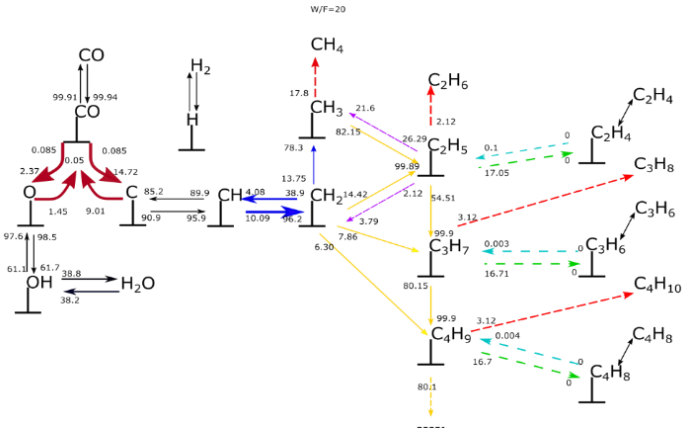

Figure 1 - Reaction path analysis on iron catalyst to produce hydrocarbons at 483 K, 1.85 kPa and 20 $kg_{cat}.s/mol_{CO}$.

As presented in Figure 1, the SEMK with RPA analysis deepens the understanding of the chemistry behind the elementary steps The findings from RPA for iron-based catalyst indicate that water forming reactions are at quasi-equilibrium, CO dissociation is kinetically relevant and the reaction rate of alkene is higher compared to alkane.

Such insight is an important step in the quest for optimal catalyst and operating condition for production of olefins via FTS

References

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